



Club de Perfumería y Cosmética

## Fichero de Datos Técnicos de Materias Primas

Situación: Materias primas-&gt;Polímeros-&gt;Carbohidratos y derivados



Salir



Subir Nivel



Bajar Nivel



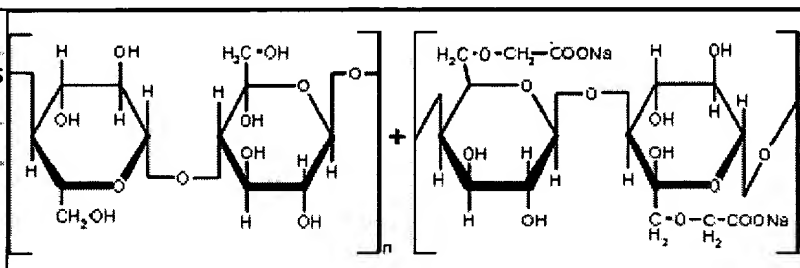
Anterior



Siguiente

Sección: Polímeros

Tipo:

Carbohidratos  
y derivados

## Microcrystalline Cellulose and Carboxymethyl Cellulose Sodium

Denominación química:

Número CAS:

## Propiedades Físico-químicas

Es un polvo blanco, inodoro, dispersable en agua. Es compatible con otros hidrocoloides y con algunos líquidos hidro-alcohólicos.

## Aplicaciones

Se usa como agente espesante y formador de suspensiones. Es además un tixótropo coloidal. Las concentraciones de uso típicas son: 1.2% en suspensiones cosméticas; 2% en suspensiones reconstituyentes; 1-2% en suspensiones farmacéuticas, y 1.5-2.5% en cremas cosméticas y lociones.

(FILE 'HOME' ENTERED AT 12:03:50 ON 01 APR 2004)

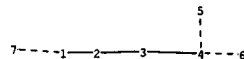
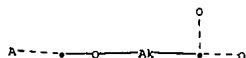
FILE 'REGISTRY' ENTERED AT 12:03:59 ON 01 APR 2004

L1               STRUCTURE UPLOADED  
L2               38 S L1 SSS SAM  
L3               6523 S L1 SSS FULL

FILE 'CAPLUS, USPATFULL, EUROPATFULL, APOLLIT, BABS, CBNB, CEN, CIN,  
DISSABS, EMA, IFIPAT, JICST-EPLUS, PASCAL, PLASNEWS, PROMT, RAPRA,  
SCISEARCH, TEXTILETECH, USPAT2, WPIDS, WTEXTILES' ENTERED AT 12:06:20 ON  
01 APR 2004

FILE 'CAPLUS, USPATFULL' ENTERED AT 12:06:50 ON 01 APR 2004

L4               1895 S L3  
L5               177 S L4 AND (POLYSACCHARIDE OR CELLULOSE OR STARCH OR GUM OR SUGAR  
L6               124 S L5 AND SOLVENT  
L7               119 S L6 AND WATER  
L8               118 S L7 AND (ALCOHOL OR ETHANOL OR METHANOL OR ISOPROPANOL)  
L9               29 S L8 AND EXTRACTION



chain nodes :

1 2 3 4 5 6 7

chain bonds :

1-2 1-7 2-3 3-4 4-5 4-6

exact/norm bonds :

1-2 1-7 2-3 3-4 4-5 4-6

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS

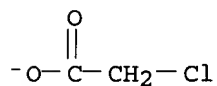
Generic attributes :

3:

Saturation : Saturated

Number of Carbon Atoms : less than 7

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 14526-03-5 REGISTRY  
 CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN 2-Chloroacetate  
 CN Chloroacetate  
 CN Chloroacetate anion  
 CN Chloroacetate ion  
 CN Chloroacetate(1-)  
 CN Chloroacetic acid ion(1-)  
 CN Monochloroacetate  
 CN Monochloroacetate ion  
 CN **Monochloroacetate ion(1-)**  
 FS 3D CONCORD  
 MF C2 H2 Cl O2  
 CI COM  
 LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS,  
 BIOTECHNO, CA, CAPLUS, CASREACT, CEN, CIN, CSCHM, CSNB, EMBASE,  
 GMELIN\*, IFICDB, IFIPAT, IFIUDB, NIOSHTIC, PIRA, PROMT, TOXCENTER,  
 TULSA, USPATFULL, VTB  
 (\*File contains numerically searchable property data)



289 REFERENCES IN FILE CA (1907 TO DATE)  
 3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 290 REFERENCES IN FILE CAPLUS (1907 TO DATE)

(FILE 'HOME' ENTERED AT 12:21:27 ON 01 APR 2004)

FILE 'REGISTRY' ENTERED AT 12:25:48 ON 01 APR 2004

E "MONCHLOROACETATE SODIUM"/CN 25

E "MONOCHLOROACETATE SODIUM"/CN 25

L1 1 S E2

FILE 'CAPLUS, USPATFULL, EUROPATFULL' ENTERED AT 12:27:43 ON 01 APR 2004

L2 298 S L1

L3 2 S L2 AND (STARCH OR CELLULOSE OR POLYSACCHARIDE OR CHITIN OR AM

L4 0 S L3 AND EXCIPIENT

L5 0 S L2 AND EXCIPIENT

L6 95 S L2 AND WATER

L7 24 S L6 AND (ALCOHOL OR ETHANOL OR ISOPROPANOL OR METHANOL)

L7 ANSWER 1 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2002:637908 CAPLUS  
 DOCUMENT NUMBER: 137:188001  
 TITLE: Viscoelastic compositions  
 INVENTOR(S): Zhou, Jian; Hughes, Trevor  
 PATENT ASSIGNEE(S): Sofitech N.V., Belg.; Schlumberger Canada Limited;  
 Schlumberger Holdings Limited; Services Petroliers  
 Schlumberger; Schlumberger Technology B.V.  
 SOURCE: PCT Int. Appl., 50 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002064945	A1	20020822	WO 2002-GB587	20020213
W:		AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM		
RW:		GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG		
GB 2372058	A1	20020814	GB 2001-3449	20010213
GB 2372058	B2	20040128		
EP 1360395	A1	20031112	EP 2002-712051	20020213
R:		AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR		
NO 2003003572	A	20031007	NO 2003-3572	20030812
PRIORITY APPLN. INFO.:			GB 2001-3449	A 20010213
			WO 2002-GB587	W 20020213

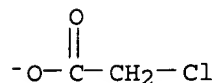
OTHER SOURCE(S): MARPAT 137:188001

AB The present invention provides aqueous viscoelastic compns. comprising a cleavable surfactant and possibly also an electrolyte. The cleavable surfactants useful in the present invention comprise at least one weak chemical bond, which is capable of being broken under appropriate conditions, to produce oil soluble and **water** soluble products typically having no interfacial properties and surface activity compared with the original surfactant mol. Further, the rheol. properties of the aqueous viscoelastic composition are usually altered upon cleavage of the cleavable surfactant generally resulting in the elimination of the viscosifying, viscoelastic and surfactant properties of the composition Aqueous viscoelastic compns. in accordance with the present invention are suitable for use in oil-field applications, particularly for hydraulic fracturing of subterranean formations. Thus, the present invention also relates to a wellbore service fluid and a method of fracturing a subterranean formation. The present invention also concerns novel cleavable surfactants.

IT 14526-03-5, 2-Chloroacetate, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (viscoelastic compns. for use as well fracturing fluids)

RN 14526-03-5 CAPLUS

CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN

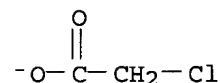
ACCESSION NUMBER: 2000:699781 CAPLUS  
DOCUMENT NUMBER: 133:362512  
TITLE: Mechanisms of Decomposition of  $\alpha$ -Hydroxydialkyl nitrosamines in Aqueous Solution  
AUTHOR(S): Mesic, Milan; Peuralahti, Jari; Blans, Patrick; Fishbein, James C.  
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Maryland Baltimore County, Baltimore, MD, 21250, USA  
SOURCE: Chemical Research in Toxicology (2000), 13(10), 983-992  
CODEN: CRTOEC; ISSN: 0893-228X  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A study of the decomposition of  $\alpha$ -hydroxydialkyl nitrosamines in aqueous 9% acetonitrile, with an ionic strength of 1 M (NaClO<sub>4</sub>), at 25 °C is reported. Plots of the logarithm of the buffer-independent rate constant,  $k_o$ , against pH are concave up and indicate a three-term rate law for the solvent reaction, including acid ( $kH^+$ )-, base ( $kOH^-$ ), and pH-independent ( $kHOH$ ) terms. Secondary  $\alpha$ -deuterium isotope effects for compound 1a, (N-nitrosomethylamino)phenylmethanol, are as follows:  $k\alpha H/k\alpha D = 1.12 \pm 0.03$  and  $1.19 \pm 0.02$  for  $kH^+$  and  $kOH^-$ , resp. General acid ( $kHA$ ) and general base ( $kA^-$ ) catalysis by more acidic carboxylic acid buffers is also observed. Structure reactivity and other parameters obtained in this study, and their changes with substrate and catalyst structure, permit the assignment of mechanisms for the  $kH^+$ ,  $kOH^-$ ,  $kHA$ , and  $kA^-$  processes. Safety: all N-nitroso compds. handled as suspect carcinogens.

IT 14526-03-5, Chloroacetate, uses  
RL: CAT (Catalyst use); USES (Uses)  
(buffer catalyst; mechanisms of decomposition of  $\alpha$ -hydroxydialkyl nitrosamines in aqueous solution)

RN 14526-03-5 CAPLUS

CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



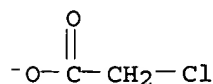
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:227504 CAPLUS  
DOCUMENT NUMBER: 122:4934  
TITLE: Electrophoresis with chemically suppressed detection  
INVENTOR(S): Dasgupta, Purnendu K.; Li-Yuan, Bao  
PATENT ASSIGNEE(S): Dow Chemical Co., USA  
SOURCE: U.S., 12 pp. Cont.-in-part of U.S. Ser. No. 764,645, abandoned.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5358612	A	19941025	US 1991-771597	19911004

CA 2096823	AA	19930325	CA 1992-2096823	19920923
CA 2096823	C	19951107		
WO 9306475	A1	19930401	WO 1992-US8071	19920923
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9226803	A1	19930427	AU 1992-26803	19920923
AU 658453	B2	19950413		
EP 558742	A1	19930908	EP 1992-920960	19920923
EP 558742	B1	19990818		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, SE				
BR 9205467	A	19931123	BR 1992-5467	19920923
JP 06501107	T2	19940127	JP 1993-506342	19920923
AT 183584	E	19990915	AT 1992-920960	19920923
CN 1073262	A	19930616	CN 1992-110852	19920924
CN 1043441	B	19990519		
KR 9707071	B1	19970502	KR 1993-71500	19930502
US 5433838	A	19950718	US 1994-258126	19940610
PRIORITY APPLN. INFO.:			US 1991-764645	B2 19910924
			US 1991-771336	A 19911004
			US 1991-771597	A 19911004
			WO 1992-US8071	A 19920923
			US 1993-143691	B1 19931028
AB	The invention provides an improved capillary electrophoresis apparatus of the type that generally includes a capillary tube, the capillary tube having a sample inlet end and an outlet end, a first electrode in elec. communication with the inlet end of the capillary tube, a second electrode in elec. communication with the outlet end of the capillary tube and a high voltage power supply in elec. communication with the first and second electrodes. The improvement is to connect a miniature ion chromatog. membrane suppressor to the outlet end of the capillary tube, to connect a conductivity detector to the membrane suppressor and to place the second electrode in the regenerant compartment of the membrane suppressor. The method embodiment of the invention for anion anal. includes the steps of: (a) separating anions of interest by capillary electrophoresis in a buffer solution; (b) exchanging cations of the buffer for regenerant cations using an ion chromatog. membrane suppressor to reduce the elec. conductivity of the buffer to produce a suppressed buffer; and (c) measuring the elec. conductivity of the suppressed buffer to determine the separated anions. Similarly, the method embodiment of the invention for cation anal. includes the steps of: (a) separating cations of interest by capillary electrophoresis in a buffer solution; (b) exchanging anions of the buffer for regenerant anions using a stationary means for exchanging anions thereby reducing the elec. conductivity of the buffer to produce a suppressed buffer; and (c) measuring the elec. conductivity of the suppressed buffer to determine the separated cations.			
IT	14526-03-5, Monochloroacetate, analysis			
	RL: ANT (Analyte); ANST (Analytical study)			
	(electrophoresis with chemical suppressed detection)			
RN	14526-03-5 CAPLUS			
CN	Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)			

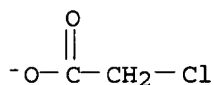


DOCUMENT NUMBER: 119:180171  
 TITLE: General base catalysis of ester hydrolysis  
 AUTHOR(S): Stefanidis, Dimitrios; Jencks, William P.  
 CORPORATE SOURCE: Grad. Dep. Biochem., Brandeis Univ., Waltham, MA, 02254-9110, USA  
 SOURCE: Journal of the American Chemical Society (1993), 115(14), 6045-50  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The hydrolysis of alkyl formates with leaving groups in the range  $pK_a = 12-16$  is catalyzed by substituted acetate anions. There is an increase in the Broensted  $\beta$  value for general base catalysis with decreasing  $pK_a$  of the leaving alc. and a complementary increase in  $-\beta_{lg}$  with decreasing  $pK_a$  of the leaving alc. and a complementary increase in  $-\beta_{lg}$  with decreasing  $pK_a$  of the catalyzing base, both of which are consistent with a value of  $\rho_{xy} = \delta\beta/-\rho K_{lg} = \delta\beta_{lg}/-\delta\rho KBH$ . simeq. 0.06. This result supports a class n mechanism of general base catalysis, in which a proton is abstracted from a nucleophilic **water** mol. by a base catalyst in the transition state; it is not consistent with the kinetically equivalent class e mechanism of electrophilic catalysis by general acids of a reaction with hydroxide ion by proton donation to the leaving alc. Solvent deuterium isotope effects in the range  $kH_2O/kD_2O = 3.6-5.3$  for a buffer-independent reaction and 2.5-2.8 for catalysis by  $CH_3COO^-$  support concerted proton transfer and O-C bond formation. The secondary isotope effect for catalysis of the hydrolysis of  $DCOOEt$  by acetate ion is  $kD/kH = 1.05$ . Both nucleophilic and general base mechanisms of catalysis by acetate anions are observed for the hydrolysis of substituted Ph formates with leaving groups of  $pK_a = 7.1-10.1$ . A small value of  $\beta = 0.12$  for general base catalysis of the hydrolysis of Ph formate and p-methylphenyl formate represents catalysis of the addition of **water** by hydrogen bonding of **water** to the base catalyst. On the other hand, a larger value of  $\beta$ , 0.35, and a decrease in  $kH_2O/kD_2O$  to 1.2 were observed for general base catalysis of the hydrolysis of p-nitrophenyl formate. It is suggested that the increase in  $\beta$  with decreasing  $\rho K_{lg}$  (an apparent anti-Hammond effect) may be accounted for by a change in mechanism, from catalysis of a stepwise reaction of Ph and p-methylphenyl formates to concerted general base catalysis of formyl transfer to **water** for the reaction of p-nitrophenyl formate.

IT 14526-03-5, Chloroacetate, uses  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalysts, for hydrolysis of formates, kinetics and mechanism of)

RN 14526-03-5 CAPLUS  
 CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 5 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1992:425674 CAPLUS  
 DOCUMENT NUMBER: 117:25674  
 TITLE: Reactions of ring-substituted 1-phenyl-2,2,2-trifluoroethyl carbocations with nucleophilic reagents: a bridge between carbocations which follow the reactivity-selectivity principle and the  $N_+$  scale  
 AUTHOR(S): Richard, John P.; Amyes, Tina L.; Vontor, Tomas  
 CORPORATE SOURCE: Dep. Chem., Univ. Kentucky, Lexington, KY, 40506-0055, USA  
 SOURCE: Journal of the American Chemical Society (1992),

114(14), 5626-34  
CODEN: JACSAT; ISSN: 0002-7863

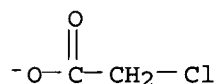
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 117:25674

AB The effect of changing carbocation reactivity on nucleophile selectivity has been determined for the reactions of ring-substituted 1-phenyl-2,2,2-trifluoroethyl carbocations,  $\text{XArCH}(\text{CF}_3)^+$ , with amines, **alcs.**, and carboxylate ions. Rate consts.,  $k_s$ , for the capture of  $\text{XArCH}(\text{CF}_3)^+$  by 50/50 (volume/volume) trifluoroethanol/water range from  $1 + 10^{10} \text{ s}^{-1}$  for 4-MeArCH(CF<sub>3</sub>)<sup>+</sup> to  $\leq 200 \text{ s}^{-1}$  for 4-Me<sub>2</sub>NArCH(CF<sub>3</sub>)<sup>+</sup>.  $\beta_{\text{nuc}} = 0.29$  Was determined for the reaction of alkylamines with 4-Me<sub>2</sub>NArCH(CF<sub>3</sub>)<sup>+</sup>.  $\beta_{\text{nuc}}$  For reaction of RCO<sub>2</sub><sup>-</sup> decreases from 0.35 for 4-Me<sub>2</sub>NArCH(CF<sub>3</sub>)<sup>+</sup> to 0.05 for 4-MeOArCH(CF<sub>3</sub>)<sup>+</sup>. This decrease is due, at least in part, to a Hammond effect on the location of the reaction transition state along the reaction coordinate.  $\beta_{\text{nuc}}$  For reaction of **alcs.** decreases from 0.48 for 4-Me<sub>2</sub>NArCH(CF<sub>3</sub>)<sup>+</sup> to 0.09 for 4-MeArCH(CF<sub>3</sub>)<sup>+</sup>. The plot of  $\log(k_{\text{EtOH}}/k_{\text{TfE}})$  for capture of  $\text{XArCH}(\text{CF}_3)^+$  by **ethanol** and trifluoroethanol against  $\log k_s$  has a shallow neg. slope for the more stable  $\text{XArCH}(\text{CF}_3)^+$ , which steepens with destabilization of the carbocation. This change in slope is due, in part, to a change in the magnitude of the Hammond effect, which corresponds to a third-derivative structure-reactivity effect,  $\text{p.thermod.yyy}' = \text{.vdelta.pyy}'/\text{-.vdelta.}\sigma > 0$ . There is considerable overlap between the reactivities of the most unstable triarylmethyl carbocations and the most stable  $\text{XArCH}(\text{CF}_3)^+$ , and there are also marked similarities in the reactivity-selectivity behavior of these species in the region of this overlap. Models are considered to explain the spectrum of reactivity-selectivity behavior that is observed on moving from very unreactive to very reactive carbocations.

IT 14526-03-5, Chloroacetate anion, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(combination of, with phenyltrifluoroethyl carbocations, kinetics and mechanism of)

RN 14526-03-5 CAPLUS

CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 6 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:542126 CAPLUS

DOCUMENT NUMBER: 115:142126

TITLE: Stability and solubilization of oxathiin carboxanilide, a novel anti-HIV agent

AUTHOR(S): Oh, Injoon; Chi, Sang Cheol; Vishnuvajjala, B. Rao; Anderson, Bradley D.

CORPORATE SOURCE: Dep. Pharm., Univ. Utah, Salt Lake City, UT, 84108, USA

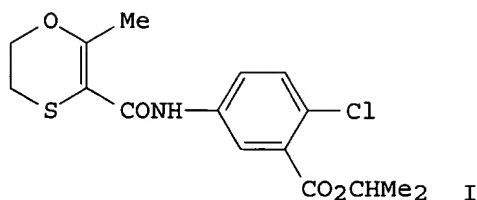
SOURCE: International Journal of Pharmaceutics (1991), 73(1), 23-31

CODEN: IJPHDE; ISSN: 0378-5173

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Oxathiin carboxanilide (NSC 615985) (I) is a novel inhibitor of HIV which is currently undergoing preclin. evaluation as an anti-AIDS agent. The purpose of this study was to generate preliminary information on the stability, degradation products, and solubility of I in order to develop prototype

parenteral dosage forms to be used in the early stages of preclin. and clin. evaluation of this candidate. A stability-indicating HPLC assay was developed for use in monitoring drug solubility and stability. The rate of degradation of I was determined in aqueous buffers as a function of pH and temperature. An

anal. of the pH-rate profile indicates that I undergoes specific acid and specific base catalyzed hydrolysis in addition to a pH-independent reaction between pH 5 and 7. The maximum shelf-life of I in aqueous solution is  $\approx 16$  days at 25°. In acid, the primary route of decomposition of I involves **water** addition to the oxathiin ring and subsequent ring-opening. In alkaline solution, ester hydrolysis predominates. The **water** solubility of I was extremely low (1.3  $\mu\text{g/mL}$ ) necessitating a search for cosolvent systems or complexing agents which would provide solubilities  $>5 \text{ mg/mL}$  for toxicol. studies. The desired solubility was achieved in 70% dimethylacetamide/**water** and 70-80% dimethylsulfoxide/**water** cosolvents. A more physiol. compatible extemporaneous lipid emulsion was also prepared containing 0.75  $\text{mg/mL}$  of I in Liposyn II 20%. The stability of I in the 20% lipid emulsion was established over a period of 48 h at 25°.

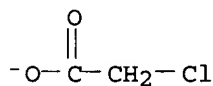
IT 14526-03-5, Chloroacetate, biological studies

RL: BIOL (Biological study)

(buffer containing, oxathiin carboxanilide degradation in, temperature effect on)

RN 14526-03-5 CAPLUS

CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 7 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:90587 CAPLUS

DOCUMENT NUMBER: 112:90587

TITLE: Cluster analysis applied to the selection and combination of buffering electrolyte systems used for capillary electrophoresis of anions with **water** or **methanol** as solvents

AUTHOR(S): Kenndler, Ernst; Gassner, Brigitte

CORPORATE SOURCE: Inst. Anal. Chem., Univ. Vienna, Vienna, A-1090, Austria

SOURCE: Analytical Chemistry (1990), 62(5), 431-6

CODEN: ANCHAM; ISSN: 0003-2700

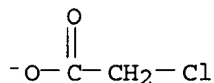
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The use of **methanol** as a solvent for buffering electrolyte systems used for the electrophoresis in capillaries was examined by cluster

anal. For this general approach, four methanolic electrolyte systems with different pH values were compared with eight aqueous systems. The similarity between these 12 systems was described by the Euclidian distances, calculated from the values of the electrophoretic mobilities of 55 anions. Clusters were constructed by use of a hierarchic algorithm and delineated by dendrograms. On the basis of the structures of the clusters, an appropriate selection is derived for the combination of electrolyte systems. It was found, that at least one methanolic system must be selected for the most favorable combination of three systems. Besides a physicochem. interpretation, the validity of the clusters was empirically proved by comparison with clusters formed by systems characterized by attributes with randomly generated values.

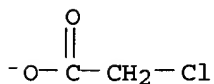
IT 14526-03-5, Chloroacetate, properties  
 RL: PRP (Properties)  
 (capillary electrophoresis of, cluster anal. for selection and  
 combination of buffering electrolyte systems for)  
 RN 14526-03-5 CAPLUS  
 CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 8 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1990:76271 CAPLUS  
 DOCUMENT NUMBER: 112:76271  
 TITLE: Relative proton transfer abilities of acids and  
 alcohols in gas phase and solutions  
 AUTHOR(S): Rakshit, S. C.; Hazra, Biren  
 CORPORATE SOURCE: Dep. Chem., Univ. Burdwan, Burdwan, 713 104, India  
 SOURCE: Proceedings - Indian Academy of Sciences, Chemical  
 Sciences (1988), 100(6), 541-7  
 CODEN: PIAADM; ISSN: 0253-4134  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The present paper applies a method, based on SCF CNDO MO charge densities and assumption of the validity of the viral theorem, for calcn. of relative proton affinities of alcs., and substituted and unsubstituted carboxylic acids in the gas phase. The paper also chalks out a path for calcn. of their relative acidities in solution phase by utilizing a solvation energy equation and binding energy data in the gas phase. The results obtained by the present method agree with ion cyclotron resonance mass spectrometric exptl. studies. The method has also been applied to cover the cases of amines in the gas phase.

IT 14526-03-5, Chloroacetate anion, properties  
 RL: PRP (Properties)  
 (binding energy of)  
 RN 14526-03-5 CAPLUS  
 CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 9 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1989:94226 CAPLUS  
 DOCUMENT NUMBER: 110:94226  
 TITLE: The significance of Broensted plots and deviations

from them in the acid- and base-catalyzed decomposition of some benzaldehyde ethyl hemiacetals and hydrates

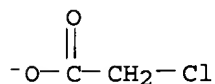
AUTHOR(S): Cox, Brian G.; Kresge, A. Jerry; Soerensen, Poul E.  
 CORPORATE SOURCE: Dep. Chem., Univ. Stirling, Stirling, FK9 4LA, UK  
 SOURCE: Acta Chemica Scandinavica, Series A: Physical and Inorganic Chemistry (1988), A42(4), 202-13  
 CODEN: ACAPCT; ISSN: 0302-4377

DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A detailed study of the general acid- and base-catalyzed decomposition of the Et hemiacetals and hydrates of three substituted benzaldehydes of different reactivity (2-chloro-5-nitrobenzaldehyde > 3-nitrobenzaldehyde > 3,4-dichlorobenzaldehyde) has been carried out at 298 K and an ionic strength of 1.0 M (KCl). Three main features are observed: (1) The change in Broensted  $\beta$  for base catalysis by carboxylate ions from  $\beta = 0.36-0.38$  for 2-chloro-5-nitrobenzaldehyde to  $\beta = 0.42-0.50$  for the corresponding reactions of 3,4-dichlorobenzaldehyde is consistent with a class n mechanism characterized by a normalized value of  $\rho_{\text{py}} = \rho_{\text{delta}}\beta / \rho_{\text{delta}}\sigma_{\text{norm}} = 0.035$ . Similarly, a change in Broensted  $\alpha$  for acid catalysis by corresponding carboxylic acids from  $\alpha = 0.33-0.39$  to  $\alpha = 0.48-0.50$  for the same compds. indicates a class e mechanism for these reactions with  $\rho_{\text{py}} = \rho_{\text{delta}}\alpha / \rho_{\text{delta}}\sigma_{\text{norm}} = 0.069$ . The correlation between  $\alpha$  and  $\sigma_{\text{norm}}$  forms two sep. lines of equal slope: one for aromatic and one for aliphatic aldehydes, presumably reflecting pronounced differences in acidities of the protonated forms of the two types of aldehydes. (2) A pos. deviation of the point for hydroxide ion catalysis from the Broensted plot decreases systematically with increasing Broensted  $\beta$  values. The change can be attributed to a variation in the balance between two concurrent mechanisms, viz. general and specific base catalysis, resp. (3) An upward curvature in the Broensted plot for base catalysis of addition to the carbonyl group might be expected in cases where  $\beta$  is relatively small. Although the catalysis was investigated in a relatively wide pK range, no sign of such a curvature in the Broensted plot was seen (within exptl. error).

IT 14526-03-5, Chloroacetate, uses and miscellaneous  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalyst, for decomposition of benzaldehyde Et hemiacetals or hydrates)

RN 14526-03-5 CAPLUS  
 CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 10 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:617098 CAPLUS  
 DOCUMENT NUMBER: 109:217098  
 TITLE: Ionic solvation in **water** + co-solvent mixtures. Part 16. Free energies of transfer of large single ions with the "neutral" component removed from **water** into **water** + **ethanol** mixtures

AUTHOR(S): Wells, Cecil F.  
 CORPORATE SOURCE: Dep. Chem., Univ. Birmingham, Edgbaston/Birmingham, B15 2TT, UK  
 SOURCE: Thermochemica Acta (1988), 130, 127-39  
 CODEN: THACAS; ISSN: 0040-6031

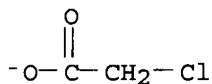
DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The method developed previously for deriving free energies of transfer of the charge only on large single ions from **water** into **water-rich water** + co-solvent mixts.  $\Delta G_t(i)c$  was applied to **water** + **ethanol** mixts. This derivation depends only on the exptl. pK values of a large acidic pos. ion producing a neutral base or of a large neutral acid producing a neg. ion and on the total free energy of transfer of the proton,  $\Delta G_t\Phi(H^+)$ . **Water** + **ethanol** was chosen for this investigations as  $\Delta G_t\Phi(H^+)$  for mole fractions of **ethanol** .apprx. 0.28-0.40 is largely independent of the assumptions used in either the spectrophotometric solvent sorting method or in the reference ion method using  $\Delta G_t\Phi(Ph_4As^+) = \Delta G_t\Phi(BPh_4^-)$ . The significance of the variation of  $\Delta G_t\Phi(i)e$  with ionic size, the sign of the charge and the extent of the distribution of the charge over the bulk of the ion in this composition range x2 .apprx. 0.28-0.40 is discussed.

IT 14526-03-5, Chloroacetate, properties  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)  
 (free energy of transfer of, in aqueous **ethanol**, calcn. of)

RN 14526-03-5 CAPLUS

CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 11 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:533830 CAPLUS

DOCUMENT NUMBER: 107:133830

TITLE: Acid- and base-catalyzed decomposition of acetaldehyde hydrate and hemiacetals in aqueous solution

AUTHOR(S): Sorensen, Poul E.; Jencks, William P.

CORPORATE SOURCE: Grad. Dep. Biochem., Brandeis Univ., Waltham, MA, 02254, USA

SOURCE: Journal of the American Chemical Society (1987), 109(15), 4675-90  
 CODEN: JACSAT; ISSN: 0002-7863

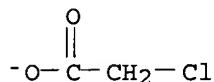
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Rate consts. and structure-reactivity parameters for general acid and general base catalysis of the reaction of acetaldehyde with **water** and **alcs.** at 25° and ionic strength 1.0 (KCl) were determined by trapping the carbonyl group formed upon cleavage of acetaldehyde hydrate or hemiacetal with semicarbazide or hydrazine. The Broensted coeffs. of  $\alpha = 0.50-0.59$  for general acid catalysts by a class e mechanism are larger than those for the corresponding reactions with formaldehyde. The difference is described by a normalized interaction coefficient  $pxy' = 0.067 = .\nu\delta\alpha.\sigma0.\nu\delta\alpha.+KHB$ . The increase in  $\alpha$  with decreasing pKa of the **alcs.** is described by the coefficient  $pxy = 0.020 = .\nu\delta\alpha.\alpha/-. \nu\delta\alpha.pKlg = .\nu\delta\alpha.\beta lg/-. \nu\delta\alpha.pKHB$ . A small increase in  $\beta lg$  for the acetaldehyde compared with formaldehyde reactions corresponds to a normalized coefficient  $pyy' = 0.014 = .\nu\delta\alpha.\beta lg/-. \nu\delta\alpha.\sigma = .\nu\delta\alpha.p/-. \nu\delta\alpha.pKlg$ . These coeffs. are consistent with a concerted reaction mechanism and a largely diagonal reaction coordinate on an energy contour diagram that is defined by the structure-reactivity parameters; there may be a larger vertical than horizontal component to the reaction coordinate. A stepwise-mechanism is excluded by a requirement for rate consts. that would have to be in the range 1013-1018 s-1 for proton transfer and for decomposition of the dipolar addition species  $R_{\pm}$ . Extrapolated rate consts. for the cleavage of  $R_{\pm}$  in the range 1020-1023 s-1 suggest that the

concerted mechanism is enforced by the absence of a significant lifetime for  $R_{\ddagger}$ . The general base catalyzed reactions show a decrease in  $\beta_{lg}$  and an increase in  $\beta$  for acetaldehyde compared with formaldehyde that correspond to  $\Delta\beta/\Delta\sigma = \Delta\rho/\Delta pK_{BH}$ . The increase in Broensted  $\beta$  values with decreasing  $pK_a$  of the leaving group and the increase in  $\beta_{lg}$  with decreasing catalyst  $pK_a$  are described by an interaction coefficient  $\rho_{xy'} = 0.07 = \Delta\beta/\Delta pK_{lg} = \Delta\beta_{lg}/\Delta pK_{BH}$  and upward curvature in the dependence of  $\log k$  on the  $pK_a$  of the leaving group (an anti-Hammond effect) is described by a value of  $\rho_{y'} = 0.20 = \Delta\beta_{lg}/\Delta pK_{lg}$ . These interaction coeffs. and a value of  $\rho_x = 0 = \Delta\beta/\Delta pK_{BH}$  from the linear Broensted plots correspond to a reaction coordinate that is rotated 57% clockwise from the vertical on an energy contour diagram that is defined by the structure-reactivity parameters, with  $\beta$  for proton transfer on the x axis. The results support a fully concerted reaction mechanism with an important component of proton transfer in the transition state. Rate consts. for the **water**-catalyzed reaction are consistent with those for buffer bases; there is no evidence for a cyclic mechanism involving proton transfer through **water**. Hydroxide ion catalysis of the reaction represents specific base catalysis. The equilibrium constant for acetaldehyde hydration was found to be  $K_h = 1.2 \pm 0.1$  at 25°C, ionic strength 1.0.

IT 14526-03-5, Chloroacetate, uses and miscellaneous  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalysts, for decomposition of acetaldehyde hemoacetals or hydrate)  
 RN 14526-03-5 CAPLUS  
 CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 12 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1987:49423 CAPLUS  
 DOCUMENT NUMBER: 106:49423  
 TITLE: How does a reaction change its mechanism? General base catalysis of the addition of **alcohols** to 1-phenylethyl carbocations  
 AUTHOR(S): Ta-Shma, Rachel; Jencks, William P.  
 CORPORATE SOURCE: Grad. Dep. Biochem., Brandeis Univ., Waltham, MA, 02254, USA  
 SOURCE: Journal of the American Chemical Society (1986), 108(25), 8040-50  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Structure-reactivity correlations are reported for general base catalysis of the addition of **alcs.** to 1-(4-dimethylamino)phenyl)ethyl and 1-(4-methoxyphenyl)ethyl carbocations in 50:40:10 H<sub>2</sub>O:CF<sub>3</sub>CH<sub>2</sub>OH:ROH. The addition of CF<sub>3</sub>CH<sub>2</sub>OH to the relatively stable [(dimethylamino)phenyl]ethyl cation is catalyzed by substituted acetate ions with  $\beta = 0.33$ , which is larger than  $\beta = 0.23$  for addition to the (methoxyphenyl)ethyl cation. Catalysis is more important for the more stable carbocation, but it decreases faster with increasing **alc.** basicity. For the H<sub>2</sub>O catalysis of **alc.** addition to 1-phenylethyl carbocations there is an increased sensitivity to the basicity of ROH with increasing carbocation stability (a Hammond effect). This indicates a small involvement of proton transfer in the transition state and is consistent with simple H-bonding of ROH to a base; it is described by a pos. interaction coefficient  $\rho_{yy'} = \delta\rho_{nuc}/\delta\sigma$ . However, for

the acetate-catalyzed reaction there is no significant increase in the sensitivity to ROH basicity with increasing carbocation stability. This represents a decrease in the  $\rho_{\text{pyy'}}$  coefficient and a shift toward the neg.  $\rho_{\text{pyy'}}$  coefficient that is expected for a fully concerted, coupled mechanism. This change in  $\rho_{\text{pyy'}}$  and other changes in interaction coeffs. describe interrelated changes in the transition state structure that accompany changes in reaction mechanism.

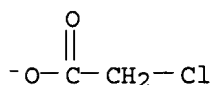
IT 14526-03-5, Chloroacetate anion, uses and miscellaneous

RL: USES (Uses)

(general-based catalysis by, of reaction of trifluoroethanol with phenylethyl carbocation derivative)

RN 14526-03-5 CAPLUS

CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 13 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1984:102488 CAPLUS

DOCUMENT NUMBER: 100:102488

TITLE: Reactions of substituted 1-phenylethyl carbocations with **alcohols** and other nucleophilic reagents

AUTHOR(S): Richard, John P.; Jencks, William P.

CORPORATE SOURCE: Grad. Dep. Biochem., Brandeis Univ., Waltham, MA, 02254, USA

SOURCE: Journal of the American Chemical Society (1984), 106(5), 1373-83

CODEN: JACSAT; ISSN: 0002-7863

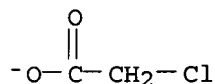
DOCUMENT TYPE: Journal

LANGUAGE: English

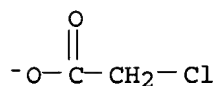
AB Selectivities of a series of substituted 1-phenylethyl carbocations toward **alcs.** and other nucleophiles have been determined by product anal. The 1-[4-(dimethylamino)phenyl]ethyl carbocation exhibits a high selectivity in its reactions with **alcs.**, with  $k_{\text{EtOH}}/k_{\text{TFE}} = 140$  and  $\beta_{\text{nuc}} = 0.5$ . The selectivity for activation-limited reactions with **alcs.** decreases progressively with increasing reactivity of the carbocation, in contrast to the behavior expected from the  $N^+$  scale of reactivity. A sharper drop in selectivity for carbocations that react faster than .apprx.  $10^9 \text{ s}^{-1}$  is attributed to an approach to limiting rate consts. for the more reactive **alc.** The limiting selectivity of  $k_{\text{EtOH}}/k_{\text{TFE}} = 2$  for carbocations with  $k_{\text{s}}$  .apprx.  $10^{11} \text{ s}^{-1}$  may represent reaction from a pool of solvent mols. in which there is a modest charge-dipole interaction between the **alc.** and carbocation. The relatively low reactivity of **water** corresponds to that expected for an **alc.** of  $\text{pK}_{\text{a}}$  .apprx. 13. This is ascribed to an imbalance between charge development and solvation of the transition state compared with  $\text{H}_3\text{O}^+$ . Substituted acetate anions react with the 1-(4-methoxyphenyl)ethyl carbocation with  $\beta_{\text{nuc}} = 0.13$ . The selectivity decreases with increasing cation reactivity as the carboxylate ions approach limiting rate consts. of .apprx.  $5 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ . This relatively low limit is attributed to a requirement for desolvation of basic oxygen anions before reaction. A dependence of solvent selectivity on the leaving group shows that the 1-(4-methylphenyl)ethyl carbocation reacts with solvent, in part, through an ion pair. Azide ion reacts from a pool that can be described by an equilibrium constant of  $K_{\text{as}} = 0.3 \text{ M}^{-1}$ . Styrene formation from this carbocation is catalyzed by a leaving carboxylate ion and by added buffers, with  $\beta = 0.14$ . The equilibrium constant for the formation of a reactive base-cation pair is .apprx.  $0.04 \text{ M}^{-1}$ . Rate consts. for collapse of the ion pair, to form ester, and for proton removal, to form

4-methylstyrene, were estimated to be approx.  $1.6 \times 10^{10} \text{ s}^{-1}$  and  $6 \times 10^7 \text{ s}^{-1}$ , resp. The rate consts. for deprotonation and for hydration of the styrene give the acid dissociation constant of the carbocation to form 4-methylstyrene,  $\text{pK}_\text{A} = -11.2$ .

IT 14526-03-5, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with phenylethyl carbocations, kinetics of)  
RN 14526-03-5 CAPLUS  
CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 14 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1977:507221 CAPLUS  
DOCUMENT NUMBER: 87:107221  
TITLE: Kinetics and mechanism of substitution of monovalent anions in  $\text{cis-[Co(en)}_2\text{X}_2\text{)]}^+$  by orthophenanthroline in **water-ethanol** mixture  
AUTHOR(S): De, G. S.; Siddhanta, S. K.  
CORPORATE SOURCE: Dep. Chem., Univ. Burdwan, Burdwan, India  
SOURCE: Journal of the Indian Chemical Society (1977), 54(1-3), 93-7  
CODEN: JICSAH; ISSN: 0019-4522  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The kinetics of replacement of monovalent anions from ethylenediamine (en) Co complexes  $\text{cis-[Co(en)}_2\text{X}_2\text{)]}^+$  ( $\text{X}^- = \text{Cl}^-$ ,  $\text{CCl}_3\text{CO}_2^-$ ,  $\text{CHCl}_2^-$ ,  $\text{CH}_2\text{ClCO}_2^-$ , and  $\text{CH}_3\text{CO}_2^-$ ) by o-phenanthroline were studied. The rate of replacement of the anions is independent of o-phenanthroline concentration and 1st order with respect to the complex concentration. The ease of displacement of the monovalent anion is  $\text{Cl}^- > \text{CCl}_3\text{CO}_2^- > \text{CHCl}_2\text{CO}_2^- > \text{CH}_2\text{ClCO}_2^- > \text{CH}_3\text{CO}_2^-$ . Lability of the outgoing anion increases as its basicity decreases. This suggests an  $\text{S}_\text{N}1$  mechanism in which bond breaking by the leaving group is important in the transition state. The effect of ionic strength on the rate and the relative magnitude of other kinetic parameters  $\Delta\text{H}^\ddagger_\text{thermod.}$  and  $\Delta\text{S}^\ddagger_\text{thermod.}$  agree with the  $\text{S}_\text{N}1$  mechanism.  
IT 14526-03-5, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(substitution reaction of, in cobalt complexes, by phenanthroline)  
RN 14526-03-5 CAPLUS  
CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 15 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1977:429615 CAPLUS  
DOCUMENT NUMBER: 87:29615  
TITLE: Solvolysis rates in aqueous-organic mixed solvents: Part II. Kinetics of alkaline solvolysis of monochloroacetate ion in **water-ethanol** solutions  
AUTHOR(S): Diefallah, E. M.; Khalil, A. M.  
CORPORATE SOURCE: Dep. Chem., Assiut Univ., Assiut, Egypt

SOURCE: Indian Journal of Chemistry, Section A: Inorganic,  
Physical, Theoretical & Analytical (1976), 14A(12),  
1012-13  
CODEN: IJCADU; ISSN: 0376-4710

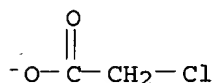
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The 2nd-order rate consts. of the alkaline solvolysis of monochloroacetate ion  
in H<sub>2</sub>O-EtOH solns. were determined. The reactivity is enhanced by increasing  
the amount of EtOH in the solvent mixts. and the rate of reaction varies  
with EtOH concentration in a nonlinear manner. The activation parameters show  
an extremum at .apprx.0.8 H<sub>2</sub>O mole fraction.

IT 14526-03-5, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(solvolysis of, in alkaline **ethanol-water** solns.,  
kinetics of)

RN 14526-03-5 CAPLUS

CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 16 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:477127 CAPLUS

DOCUMENT NUMBER: 85:77127

TITLE: Solvolysis rates in aqueous-organic mixed solvents.  
III. Kinetics of the alkaline solvolysis of  
monochloroacetate ion in **water-tert-butyl**  
**alcohol** solutions

AUTHOR(S): Diefallah, El-Hussieny M.

CORPORATE SOURCE: Dep. Chem., Assiut Univ., Assiut, Egypt

SOURCE: Canadian Journal of Chemistry (1976), 54(11), 1687-91  
CODEN: CJCHAG; ISSN: 0008-4042

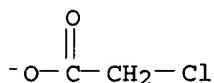
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The rate of alkaline solvolysis of ClCH<sub>2</sub>CO<sub>2</sub><sup>-</sup> in H<sub>2</sub>O-Me<sub>3</sub>COH is 1st order in  
ClCH<sub>2</sub>CO<sub>2</sub><sup>-</sup> and is total solvoxide ion concentration. The reactivity is enhanced,  
first slowly, and then more rapidly, by increasing the concentration of Me<sub>3</sub>COH.  
The rate of reaction increases with the reciprocal of the dielec. constant  
of the medium. The activation parameters ΔH\* and ΔS\* show a  
min. at .apprx.0.9 H<sub>2</sub>O mole fraction. The electrostatic theory and the  
changing of solvent structure is discussed.

IT 14526-03-5, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(solvolysis in **water-tert-butyl alc.**, kinetics of)

RN 14526-03-5 CAPLUS

CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 17 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1975:42570 CAPLUS

DOCUMENT NUMBER: 82:42570

TITLE: Solvolysis rates in aqueous-organic mixed solvents.  
I. Kinetics of alkaline solvolysis of

monochloroacetate ion in **water-methanol** solutions

AUTHOR(S): Azzam, Ahmed M.; Diefallah, El-Hussieny M.  
CORPORATE SOURCE: Ain Shams Univ., Cairo, Egypt  
SOURCE: Zeitschrift fuer Physikalische Chemie (Muenchen, Germany) (1974), 91(1-4), 44-53  
CODEN: ZPCFAX; ISSN: 0044-3336

DOCUMENT TYPE: Journal  
LANGUAGE: English

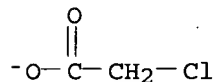
AB The kinetics of the alkaline solvolysis of ClCH<sub>2</sub>CO<sub>2</sub><sup>-</sup> (I, as Na salt) in (0-100%) H<sub>2</sub>O-MeOH solns. at 0.1-0.2M NaOH, and 0.02-0.1M I showed overall 2nd order dependence and 1st order with respect to I and NaOH. The reaction rates increased with increasing MeOH concentration up to a maximum at

0.85 mole fraction MeOH, and the activation parameters passed through a min. at 0.7 mole fraction H<sub>2</sub>O.

IT 14526-03-5, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(alkaline hydrolysis and methanolysis of, kinetics of)

RN 14526-03-5 CAPLUS

CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 18 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1971:68217 CAPLUS

DOCUMENT NUMBER: 74:68217

TITLE: Kinetics of the alkaline solvolysis of monochloroacetate ions in **methanol-water** mixture at 50-95.deg.

AUTHOR(S): Koehler, Wolfram; Neuheiser, Lothar  
CORPORATE SOURCE: Sekt. Verfahrenchem., Tech. Hochsch. Chem. Carl Schorlemmer, Leuna-Merseburg, Fed. Rep. Ger.  
SOURCE: Zeitschrift fuer Physikalische Chemie (Leipzig) (1970), 245(3-4), 272-4  
CODEN: ZPCLAH; ISSN: 0323-4479

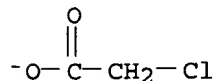
DOCUMENT TYPE: Journal  
LANGUAGE: German

AB In the alkaline solvolysis of the ClCH<sub>2</sub>CO<sub>2</sub><sup>-</sup> ion in MeOH-H<sub>2</sub>O mixts., the following reactions occur: (1) ClCH<sub>2</sub>CO<sub>2</sub><sup>-</sup> + OHOH → HOCH<sub>2</sub>CO<sub>2</sub><sup>-</sup> + Cl<sup>-</sup>, and (2) ClCH<sub>2</sub>CO<sub>2</sub><sup>-</sup> + OMe-OMe → MeOCH<sub>2</sub>CO<sub>2</sub><sup>-</sup> + Cl<sup>-</sup>. By determination of the chloride and methoxyacetate ion concentration, the apparent rate consts. of (1) and (2) were determined and are listed as functions of temperature and composition of the solns.

IT 14526-03-5, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(solvolysis of, kinetics of alkaline **methanol-water**)

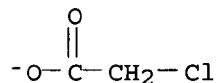
RN 14526-03-5 CAPLUS

CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 19 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1970:407768 CAPLUS  
 DOCUMENT NUMBER: 73:7768  
 TITLE: Kinetics of the iodination of some nitroalkanes in  
**methanol-water** and tert-butyl  
**alcohol-water** mixtures  
 AUTHOR(S): Tenno, T.; Talvik, A.  
 CORPORATE SOURCE: Tartu State Univ., Tartu, USSR  
 SOURCE: Reaktsionnaya Sposobnost Organicheskikh Soedinenii  
 (1969), 6(3), 882-9  
 CODEN: RSOTAY; ISSN: 0375-9520  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 AB The rates of ionization of MeNO<sub>2</sub>, EtNO<sub>2</sub>, and iso-PrNO<sub>2</sub> were studied by  
 studying the kinetics of iodination in the presence of the chloroacetate  
 ion in MeOH-H<sub>2</sub>O and tert-BuOH-H<sub>2</sub>O mixts. The nonlinearity of log K-NROH  
 and log K-(D - 1)/(2D + 1) dependences, where K is rate of ionization  
 constant, NROH is molar fraction of the alc., and D is dielec.  
 constant, indicated that sp. solvation contributes substantially to the  
 total solvent effect.  
 IT 14526-03-5, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (with nitroalkanes, in alc. solution)  
 RN 14526-03-5 CAPLUS  
 CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 20 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1970:48019 CAPLUS  
 DOCUMENT NUMBER: 72:48019  
 TITLE: Kinetics of alkaline hydrolysis of the  
 monochloroacetate ion in acetone-, 1,4-dioxane-,  
 tetrahydrofuran-, dimethylsulfoxide-, and  
**methanol-water** mixtures  
 AUTHOR(S): Koehler, Wolfram; Neuheiser, Lothar  
 SOURCE: Wissenschaftliche Zeitschrift der Technischen  
 Hochschule fuer Chemie Carl Schorlemmer  
 Leuna-Merseburg (1969), 11(3), 232-5  
 CODEN: WZTLA3; ISSN: 0043-6909  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 AB The reactions were studied of 0.1M OH- and 0.1M ClCH<sub>2</sub>COO- as a function  
 of the solvent mixture in sealed ampuls at 50-95°. The decrease of  
 the OH- concentration corresponded to the increase in the Cl- concentration  
 During the  
 kinetic investigations in alkaline MeOH-H<sub>2</sub>O mixts., the formation of  
 methoxyacetate ions was taken into consideration. These ions were determined  
 by the Zeisel-Vieboeck method. The rate consts. were comparable for the  
 reactions: ClCH<sub>2</sub>COO- + OH- → HOCH<sub>2</sub>COO- + Cl-, and ClCH<sub>2</sub>COO- +  
 MeO- → MeOCH<sub>2</sub>COO- + Cl-. The ratio of the glycolate and  
 methoxyacetate ions formed was determined. The results obtained permitted sep.  
 determination of the rate consts. for the alkaline hydrolysis of the  
 chloroacetate  
 ions. Up to conversion degrees of 60-70%, the title reaction followed a  
 2nd order law. The dependence was investigated of the alkaline hydrolysis  
 rate constant on the composition of the binary solvent mixture. The increase  
 of the  
 rate constant with increasing content of aprotic solvent was accounted for.  
 The dependence of the rate consts. and the activation parameters on the

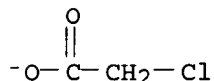
solvent composition was discussed, on the basis of different solvation of the basic, and transition states.

IT 14526-03-5, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrolysis of, by hydroxide, solvent effects on)

RN 14526-03-5 CAPLUS

CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 21 OF 24 USPATFULL on STN

ACCESSION NUMBER: 94:92992 USPATFULL

TITLE: Electrophoresis with chemically suppressed detection

INVENTOR(S): Dasgupta, Purnendu K., Lubbock, TX, United States

Li-Yuan, Bao, Lubbock, TX, United States

PATENT ASSIGNEE(S): The Dow Chemical Company, Midland, MI, United States  
(U.S. corporation)

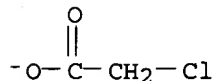
	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5358612		19941025
APPLICATION INFO.:	US 1991-771597		19911004 (7)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 1991-764645, filed on 24 Sep 1991, now abandoned		
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	Granted		
PRIMARY EXAMINER:	Niebling, John		
ASSISTANT EXAMINER:	Starsiak, Jr., John S.		
LEGAL REPRESENTATIVE:	Stevens, Timothy S., Halldorson, Burke M.		
NUMBER OF CLAIMS:	2		
EXEMPLARY CLAIM:	1		
NUMBER OF DRAWINGS:	6 Drawing Figure(s); 3 Drawing Page(s)		
LINE COUNT:	794		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Improved capillary electrophoresis apparatus of the type that generally includes a capillary tube, the capillary tube having a sample inlet end and an outlet end, a first electrode in electrical communication with the inlet end of the capillary tube, a second electrode in electrical communication with the outlet end of the capillary tube and a high voltage power supply in electrical communication with the first and second electrodes. The improvement is to connect a miniature Ion Chromatography membrane suppressor to the outlet end of the capillary tube, to connect a conductivity detector to the membrane suppressor and to place the second electrode in the regenerant compartment of the membrane suppressor. The method embodiment of the invention for anion analysis includes the steps of: (a) separating anions of interest by capillary electrophoresis in a buffer solution; (b) exchanging cations of the buffer for regenerant cations using an ion chromatography membrane suppressor to reduce the electrical conductivity of the buffer to produce a suppressed buffer; and (c) measuring the electrical conductivity of the suppressed buffer to determine the separated anions. Similarly, the method embodiment of the invention for cation analysis includes the steps of: (a) separating cations of interest by capillary electrophoresis in a buffer solution; (b) exchanging anions of the buffer for regenerant anions using a stationary means for exchanging anions thereby reducing the electrical conductivity of the buffer to produce a suppressed buffer; and (c) measuring the electrical conductivity of the suppressed buffer to determine the separated cations.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 14526-03-5, Monochloroacetate, analysis  
(electrophoresis with chemical suppressed detection)  
RN 14526-03-5 USPATFULL  
CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 22 OF 24 USPATFULL on STN

ACCESSION NUMBER: 83:52715 USPATFULL  
TITLE: Ion exchange chromatography with indirect photometric detection  
INVENTOR(S): Small, Hamish, Midland, MI, United States  
Miller, Jr., Theodore E., Midland, MI, United States  
PATENT ASSIGNEE(S): The Dow Chemical Company, Midland, MI, United States  
(U.S. corporation)

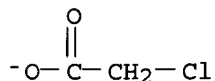
	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4414842		19831115
APPLICATION INFO.:	US 1982-364705		19820402 (6)
RELATED APPLN. INFO.:	Continuation of Ser. No. US 1980-153814, filed on 27 May 1980, now abandoned		
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	Granted		
PRIMARY EXAMINER:	Myracle, Jerry W.		
LEGAL REPRESENTATIVE:	Halldorson, Burke M.		
NUMBER OF CLAIMS:	20		
EXEMPLARY CLAIM:	1		
NUMBER OF DRAWINGS:	16 Drawing Figure(s); 5 Drawing Page(s)		
LINE COUNT:	987		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB An improved technique for the measurement of ions in solution where the ions of interest are chromatographically displaced from an ion exchange column by an eluting ion which is or is made light-absorbing, and where the eluted sample ions, which are transparent (at the monitored wavelength), are detected and quantified from the decrements they cause in effluent absorbance as revealed by photometric monitoring.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 14526-03-5, analysis  
(ion-exchange chromatog. of, indirect spectrophotometry detection in)  
RN 14526-03-5 USPATFULL  
CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 23 OF 24 USPATFULL on STN

ACCESSION NUMBER: 75:68437 USPATFULL  
TITLE: Method and apparatus for quantitative chromatographic analysis of cationic species  
INVENTOR(S): Stevens, Timothy S., Midland, MI, United States  
PATENT ASSIGNEE(S): The Dow Chemical Company, Midland, MI, United States

(U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 3926559		19751216
APPLICATION INFO.:	US 1973-386262		19730806 (5)
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	Granted		
PRIMARY EXAMINER:	Wolk, Morris O.		
ASSISTANT EXAMINER:	Marantz, Sidney		
LEGAL REPRESENTATIVE:	Schilling, Edward E.		
NUMBER OF CLAIMS:	17		
EXEMPLARY CLAIM:	1		
NUMBER OF DRAWINGS:	1 Drawing Figure(s); 1 Drawing Page(s)		
LINE COUNT:	963		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Apparatus and method for chromatographic quantitative analysis of a plurality of species of cations in sample solution. A sample of the solution is added to a first ion exchange resin bed charged with a cation exchange resin and the sample eluted therefrom with a solution of mixed developing reagent consisting of either soluble silver salts or soluble barium salts and compatible, i.e., non-precipitating acid, the cations being chromatographically separated upon such elution. The effluent from the first ion exchange resin bed is passed through a second ion exchange resin bed charged with an anion exchange resin in an appropriate form to precipitate the silver salt or barium salt used in the developing reagent. As elution continues the sample passes from the second ion exchange resin bed to a third ion exchange resin bed charged with an anion exchange resin in the hydroxide form. Precipitation of developing reagents in the second bed and neutralization of acid in the third bed are carried out without interfering with the ionic separations achieved in the first bed. Each separated cationic species is quantitatively sensed by a detector such as a conductivity cell on exiting from the third ion exchange resin bed.

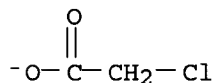
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 14526-03-5, analysis

(separation and determination of, by ion-exchange chromatog. on dual-resin columns)

RN 14526-03-5 USPATFULL

CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 24 OF 24 USPATFULL on STN

ACCESSION NUMBER: 75:62244 USPATFULL

TITLE: Apparatus and method for quantitative analysis of ionic species by liquid column chromatography

INVENTOR(S): Small, Hamish, Midland, MI, United States  
Bauman, William C., Lake Jackson, TX, United States

PATENT ASSIGNEE(S): The Dow Chemical Company, Midland, MI, United States  
(U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 3920397		19751118
APPLICATION INFO.:	US 1973-386260		19730806 (5)
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	Granted		

PRIMARY EXAMINER: Wolk, Morris O.  
ASSISTANT EXAMINER: Marantz, Sidney  
LEGAL REPRESENTATIVE: Schilling, Edward E.  
NUMBER OF CLAIMS: 58  
EXEMPLARY CLAIM: 1  
NUMBER OF DRAWINGS: 4 Drawing Figure(s); 2 Drawing Page(s)  
LINE COUNT: 1112

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Apparatus and method for the chromatographic quantitative analysis of a solution containing a plurality of ions. In a particular analysis, the assay is limited to determining either solely the cations or solely the anions. A sample of the solution is added to a first ion exchange bed and eluted therefrom with a solution of developing reagent. The effluent from the first ion exchange bed is passed through a second ion exchange bed where the developing reagent is converted to a weakly ionized form and the ions of interest are paired with a common ion of the opposite sign without destroying the ionic separation produced by the first ion exchange bed. Each separated ionic species of the preselected common sign is quantitatively sensed by a detector, such as a conductivity cell, on exiting from the second ion exchange bed.

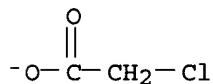
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 14526-03-5, analysis

(separation and determination of, by ion-exchange chromatog. on dual-resin columns)

RN 14526-03-5 USPATFULL

CN Acetic acid, chloro-, ion(1-) (8CI, 9CI) (CA INDEX NAME)



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